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CONVERGENCE OF THE QR ALGORITHM

by

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ABSTRACT

The QR algorithm of J. G. F. Francis is used in computing matrix eigenvalues. The convergence proof given here is an analogue of Rutishauser's proof of the convergence of the LR algorithm.

CONVERGENCE OF THE QR ALGORITHM

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1. Introduction

J. G. F. Francis presented his QR transformation in 1961 in two articles [1]. We give here a new proof of the main result, namely Theorem 3 in [1].

Francis proposed an algorithm for generating from a given square matrix a sequence of unitarily similar matrices. He proved that if the eigenvalues have distinct moduli then, in the limit, the form of the matrices is triangular and, although the sequence may not converge in the strict sense, the diagonal elements do tend to the eigenvalues.

In practice an elegant modification of the basic algorithm provides a speedy and stable method for calculating matrix eigenvalues on a digital computer. In this paper we shall be concerned only with the basic algorithm.

The QR transformation is an analogue of the LR transformation of Rutishauser [2]. Although it is more complicated technically, our convergence proof is an analogue of Rutishauser's convergence proof for the LR transformation. The convergence rate emerges naturally

in the course of the proof.

In the next section we describe those properties of the QR transformation which are essential for our proof. The author would like to thank Eugene Isaacson for helpful suggestions on the presentation of the argument.

2. The QR Transformation

From the original matrix A $(=A^{(1)})$, assumed non-singular, a sequence $A^{(k)}$ is produced as follows. At the k^{th} stage $A^{(k)}$ is decomposed into a product of a unitary matrix $Q^{(k)}$ by an upper (or right) triangular matrix $R^{(k)}$. Then $A^{(k+1)}$ is formed by post multiplying $R^{(k)}$ by $Q^{(k)}$. The factorization is always possible by Theorem 1 in [1] and can be accomplished in a stable manner. By requiring that the diagonal elements of $R^{(k)}$ be positive the decomposition becomes unique. Thus

$$A^{(1)} = A$$

(21) $$A^{(k)} = Q^{(k)}R^{(k)}\ , \quad A^{(k+1)} = R^{(k)}Q^{(k)}\ , \quad k = 1,2,\ldots$$

It follows from these definitions that

(22) $$A^{(k+1)} = Q^{(k)*}Q^{(k-1)*}\ldots Q^{(1)*}AQ^{(1)}\ldots Q^{(k-1)}Q^{(k)}$$

where M^* denotes the conjugate transpose of M. Following

Francis we write

$$P^{(k)} = Q^{(1)}Q^{(2)}\ldots Q^{(k)} \quad \text{and} \quad S^{(k)} = R^{(k)}R^{(k-1)}\ldots R^{(1)} \ .$$

Thus the $P^{(k)}$ are unitary and the $S^{(k)}$ are upper triangular. It can be verified, by using (21) repeatedly, that

$$P^{(k)}S^{(k)} = A^k \ . \tag{23}$$

Equations (22) and (23) together give the following useful result.

THEOREM 2 (Francis). <u>If</u> A <u>is non-singular then</u> $A^{(k+1)} = P^{(k)*}AP^{(k)}$ <u>where</u> $P^{(k)}S^{(k)}$ <u>is the unitary-triangular decomposition of</u> A^k .

Thus to prove the convergence of $\left\{A^{(k)}\right\}$ as $k \to \infty$ it suffices to prove the convergence of $\left\{P^{(k)}\right\}$.

3. <u>Determinantal Representation of Q .</u>

The unitary-triangular, or QR , factorization of any non-singular matrix M is mathematically equivalent to the Gram-Schmidt process for orthonormalising the linearly independent columns of M . The usual process amounts to post multiplying the matrix M by an upper triangular matrix, actually R^{-1} , to obtain a unitary

matrix Q. The usual normalisation invoked to give uniqueness to the Gram-Schmidt process is precisely the requirement that R have positive diagonal elements, see [3]. Only when there is need to stress the dependence of Q and R on M will we write $Q = Q(M)$, $R = R(M)$.

In the proofs which follow we shall use the following notation. The j^{th} column of a matrix M is m_j, except for the identity matrix whose j^{th} column is denoted by e_j. Let $\delta_j(M)$ denote the leading principal $j \times j$ minor (determinant) of M and let $\gamma_j(M) = \delta_j(M^*M)$. If M is $n \times n$ then $\gamma_n(M)$ is the Gramian (determinant) of M. Let $\widetilde{m}_j$ be the vector obtained by replacing the numbers in the last row of $\gamma_j(M)$ by the vectors $m_1, m_2, \ldots m_j$. Thus

$$\gamma_j(M) = \det \begin{bmatrix} m_1^* m_1 & \cdots & m_1^* m_j \\ \vdots & & \vdots \\ m_j^* m_1 & \cdots & m_j^* m_j \end{bmatrix} , \quad \gamma_0 = 1 ,$$

$$\widetilde{m}_j = \det \begin{bmatrix} m_1^* m_1 & \cdots & m_1^* m_j \\ \vdots & & \vdots \\ m_{j-1}^* m_1 & \cdots & m_{j-1}^* m_j \\ m_1 & \cdots & m_j \end{bmatrix}$$

By expanding the latter determinant formally with respect to the last row we see that $\widetilde{m}_j$ is a linear combination of $m_1, m_2, \ldots, m_j$.

Now suppose that $M = QR$. With the notation given above we can give a determinantal representation for q_j (the j^{th} column of Q). This result is given by Szegö in [3].

LEMMA 1

$$q_j = (\gamma_j(M)\gamma_{j-1}(M))^{-\frac{1}{2}}\tilde{m}_j . \tag{31}$$

The lemma follows from the observation that $\tilde{m}_j$ is orthogonal to $m_1,\ldots,m_{j-1}$ and that $\tilde{m}_j^*\tilde{m}_j = \gamma_j(M)\gamma_{j-1}(M)$. This lemma is the tool for our convergence proof.

A representation for the i th element of $\tilde{m}_j$ will prove convenient. For a given value of j denote by $M_{i,j}$ the matrix M with m_j replaced by e_i, then

$$e_i^*\tilde{m}_j = \delta_j(M_{i,j}^*M) . \tag{32}$$

4. A lemma on determinants

We shall need to know the form of the determinant of a certain product of matrices. Let $Z_n = \{1,\ldots,n\}$ and let $Z_{n,k}$ be the set of all strictly increasing sequences of k elements chosen from the set Z_n.

LEMMA 2. *Let* A,L,B,M,C *be* $n \times n$ *matrices,* L *and* M *diagonal. Then*

$$(41)\quad \delta_k(ALBMC) = \sum_{\sigma,\rho\in Z_{n,k}} g^{\sigma,\rho}(\ell_{\sigma_1}\cdots\ell_{\sigma_k})(m_{\rho_1}\cdots m_{\rho_k}) .$$

Proof. For $\alpha,\beta\in Z_{n,k}$ and E an $n\times n$ matrix let E^{α}_{β} be the submatrix obtained by selecting from E rows $\alpha_1,\ldots,\alpha_k$ and columns $\beta_1,\ldots,\beta_k$. Let $\underline{k} = (1,2,\ldots,k)$, then by the theory of determinants,

$$\det(E^{\underline{k}}LF_{\underline{k}}) = \sum_{\alpha\in Z_{n,k}} \det(E^{\underline{k}}_{\alpha})\det((LF)^{\alpha}_{\underline{k}})$$

$$= \sum_{\alpha\in Z_{n,k}} \det(E^{\underline{k}}_{\alpha})\det(F^{\alpha}_{\underline{k}})(\ell_{\alpha_1}\cdots\ell_{\alpha_k}) .$$

Two applications of this formula gives the result of the lemma with

$$(40)\qquad g^{\sigma,\rho} = \det(A^{\underline{k}}_{\sigma})\det(B^{\sigma}_{\rho})\det(C^{\rho}_{\underline{k}}) .$$

COROLLARY. <u>If the</u> k^{th} <u>row of</u> A is e^*_k <u>then</u> ℓ_k <u>is a factor of</u> $\delta_k(ALBMC)$.

Proof. For all $\sigma\in Z_{n,k}$, $k\notin\sigma$ implies that row k of $A^{\underline{k}}_{\sigma}$ is null. Thus the coefficients $g^{\sigma,\rho}$ in (40) vanish unless the term involves ℓ_k . Q. E. D.

5. <u>Convergence of the algorithm.</u>

In Section 2 we saw that the QR algorithm when

applied to any non-singular $n \times n$ matrix $A = A^{(1)}$ produces a sequence $\{A^{(k)}\}$ in which $A^{(k+1)} = P^{(k)*}AP^{(k)}$ and $P^{(k)}$ is the unitary factor of $M = A^k$; i.e. $P = P^{(k)} = Q(A^k)$. Equations (31) and (32) of Section 3 applied to M give a representation of a typical element of P .

$$(50) \qquad p_{ij} = e_i^* p_j = \frac{\delta_j(M_{i,j}^* M)}{[\gamma_j(M)\gamma_{j-1}(M)]^{1/2}} ,$$

where $\gamma_j(B) = \delta_j(B^*B)$, the leading principal $j \times j$ minor of B^*B , and $M_{i,j}$ is M with column j replaced by e_i .

To exhibit the conceptual simplicity of the proof of Francis' Theorem 3 we consider first the special case of well-ordered eigenvalues.

THEOREM 3. _Let_ $A = X\Lambda Y$ _where_ $Y = X^{-1}$, $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$.

_If_ (i) $|\lambda_1| > |\lambda_2| > \ldots > |\lambda_n| > 0$,

and (ii) $\delta_\nu(Y) \neq 0$, $\nu = 1, \ldots, n$,

then, as $k \to \infty$, _the elements of_ $A^{(k)}$ _below the principal diagonal tend to zero, the moduli of those above tend to fixed values, and_ $a_{ii}^{(k)} \to \lambda_i$, $i = 1, \ldots, n$.

Proof. We examine first the denominator of (50). Now

$\gamma_j(M) = \delta_j(Y^* \bar{\Lambda}^k X^* X \Lambda^k Y)$ and by Lemma 2 this is a sum of terms of the form

(51) $$\overline{\xi(\lambda_{\sigma_1} \cdots \lambda_{\sigma_j})}^{k} (\lambda_{\rho_1} \cdots \lambda_{\rho_j})^{k} \quad ,$$

$\sigma, \rho \in Z_{n,j}$ and ξ depends on σ and ρ but not on k .
Hence, by (i) ,

(52) $$\gamma_j(M) \sim \xi_j |\lambda_1 \cdots \lambda_j|^{2k}\left(1+O(r_j^k)\right) \;, \quad k \to \infty \;,$$

provided that $\xi_j \neq 0$, where $r_j = |\lambda_{j+1}/\lambda_j|$, $r_o = r_n = 0$.
From equation (40) we have

(53) $$\xi_j = \gamma_j(X)|\delta_j(Y)|^2 > 0$$

since $\gamma_j(X)$ is the Gram determinant of j of the linearly independent columns of X and $\delta_j(Y) \neq 0$ by (ii) .

To examine the numerator of (50) we observe that

(54) $$M_{i,j} = X_{i,j} \Lambda^k_{j,j} Y_{j,j}$$

Thus $\delta_j(M^*_{i,j} M) = \delta_j(Y^*_{j,j} \bar{\Lambda}^k_{j,j} X^*_{i,j} X \Lambda Y)$ and may be expanded as a sum of terms of the form given in (51). However row j of $Y^*_{j,j}$ is e^*_j and so, by the corollary of Lemma 2, each non-zero term in the expansion includes the

(j,j) element of $\bar{\Lambda}^k_{j,j}$, which is 1, and hence involves only $j-1$ factors $\bar{\lambda}^k_\nu$, $\nu \neq j$. Thus $\delta_j(M_{i,j}{}^*M)$ is a sum of terms of the form

$$(55) \qquad \eta\,\overline{(\lambda_{\tau_1}\cdots\lambda_{\tau_{j-1}})}^{\,k}\,(\lambda_{\rho_1}\cdots\lambda_{\rho_j})^k \quad ,$$

where $\rho \in Z_{n,j}$, $\tau \in Z_{n,j-1}$ with $j \notin \tau$, and $\eta = \eta(\tau,\rho)$ does not depend on k. Hence by (i), as $k \to \infty$,

$$(56) \qquad \delta_j(M_{i,j}{}^*M) \sim \eta_{i,j}\,|\lambda_1\cdots\lambda_{j-1}|^{2k}\lambda_j^k\left(1+0(r_j{}^k)\right) \quad ,$$

provided that $\eta_{i,j} \neq 0$. From equation (40) we have

$$(57) \qquad \eta_{i,j} = \overline{\delta_{j-1}(Y)}\,\delta_j(X_{i,j}{}^*X)\,\delta_j(Y) \quad .$$

If $\delta_j(M_{i,j}{}^*M) \neq 0$ then $\eta_{i,j} \neq 0$, by (ii), and we may substitute (52) and (56) into (50) to obtain

$$(58) \qquad p_{ij}^{(k+1)} \sim \frac{\eta_{ij}}{(\xi_{j-1}\xi_j)^{1/2}}\left(\frac{\lambda_j}{|\lambda_j|}\right)^k\left(1 + 0(r_j^k) + 0(r_{j-1}^k)\right) .$$

By comparing (53) and (57) with (31) and (32) we find

$$(59) \qquad \frac{\eta_{ij}}{(\xi_{j-1}\xi_j)^{1/2}} = \frac{\operatorname{sgn}\delta_j(Y)}{\operatorname{sgn}\delta_{j-1}(Y)}\; q_{ij}(X) \quad ,$$

where $q_{ij}(X)$ is the (i,j) element of $Q = Q(X)$. By (ii) we note that if $\eta_{ij} = 0$ then $q_{ij}(X) = 0$ and, though (58) fails, $p_{ij}^{(k)} \to 0$. Thus whatever the value of η_{ij} we have, as $k \to \infty$,

$$(60) \qquad |p_{ij}^{(k+1)}| \to q_{ij}(X); \quad i,j = 1,\ldots,n .$$

Since the signa in (58) and (59) do not depend on i and since $X = QR$ we have, as $k \to \infty$,

$$|a_{ij}^{(k+1)}| = | \sum_{\alpha, \beta = 1}^{n} a_{\alpha\beta} \bar{p}_{\alpha i}^{(k)} p_{\beta j}^{(k)}|$$

$$(61) \qquad \to | \sum_{\alpha, \beta = 1}^{n} a_{\alpha\beta} \bar{q}_{\alpha i} q_{\beta j}| = |(Q^* AQ)_{ij}| = |(R \Lambda R^{-1})_{ij}| ,$$

$$a_{jj}^{(k+1)} = \sum_{\alpha, \beta = 1}^{n} a_{\alpha\beta} \bar{p}_{\alpha j}^{(k)} p_{\beta j}^{(k)}$$

$$(62) \qquad \to \sum_{\alpha, \beta = 1}^{n} a_{\alpha\beta} \bar{q}_{\alpha j} q_{\beta j} = (Q^* AQ)_{jj} = (R \Lambda R^{-1})_{jj} = \lambda_j .$$

This proves Theorem 3 since R is upper triangular.

6. Convergence of the algorithm with disorder of the eigenvalues.

We now show how the proof of Theorem 3 may be carried

over with almost no alteration for any non-singular matrix with eigenvalues of distinct modulus. The key is to keep hypothesis (ii) at the expense of (i) .

For any A the canonical form $A = X\Lambda Y$ is unique only up to a permutation $P\Lambda P^{-1}$ of Λ and the corresponding permutations in the columns of X and the rows of Y . We now relabel the elements of Λ so that for $\nu = 1, \ldots, n$; $\delta_\nu(Y) \neq 0$ and $\lambda_\nu (= \Lambda_{\nu\nu})$ is an eigenvalue of maximal modulus such that this is so. Since Y is non-singular this relabelling is always possible.

We need two lemmas to show that with this new labelling the dominant terms among those of the form (51) and (55) are given by the same expressions as before, namely (52) and (56).

We recall that if $\sigma, \rho \in Z_{n,j}$ then Y_ρ^σ denotes the $j \times j$ submatrix involving rows $\sigma_1, \ldots, \sigma_j$ and $\rho_1, \ldots, \rho_j$ of the $n \times n$ matrix Y . Also $\underline{j} = (1, \ldots, j)$.

For given i, j , the coefficients ξ and η in (51) and (55) are given by equation (40) as

$$\xi(\sigma,\rho) = \det(\bar{Y}_{\underline{j}}^{\sigma}) \det\left[(X^* X)_\rho^\sigma\right] \det(Y_{\underline{j}}^{\rho}) \quad ,$$

$$\eta(\tau,\rho) = \det(\bar{Y}_{\underline{j-1}}^{\tau}) \det\left[(X_{i,j}{}^* X)_\rho^\tau\right] \det(Y_{\underline{j}}^{\rho}) \quad ,$$

where $\sigma, \rho, \tau' \in Z_{n,j}$, $\tau \in Z_{n,j-1}$, $j \notin \tau$, τ' is τ supplemented with j. From these expressions it is clear that if $|\lambda_{\rho_1} \ldots \lambda_{\rho_j}| > |\lambda_1 \ldots \lambda_j|$ implies $\det(\underline{Y}_j^{\rho}) = 0$ then all terms which might dominate $\xi_j |\lambda_1 \ldots \lambda_j|^{2k}$ and $\eta_{ij} |\lambda_1 \ldots \lambda_{j-1}|^{2k} \lambda_j$ as $k \to \infty$ will, in fact, have zero coefficients.

LEMMA 3. *Let* $V = \{v_i : i = 1, \ldots, k+1\}$ *be a set of any* $k+1$ *k-dimensional vectors. Then the subset* U *of those* v_i *such that the remaining vectors are linearly independent is either empty or linearly dependent.*

Proof. If U is not empty then v_{k+1} (say) $\in U$. $v_{k+1} = \sum_{i=1}^{k} \alpha_i v_i$ with unique coefficients α_i. If $U = V$ then U is clearly linearly dependent. If v_1 (say) $\notin U$ then $\{v_2, \ldots, v_{k+1}\}$ is dependent whilst $\{v_2, \ldots, v_k\}$ is independent since $v_{k+1} \in U$. Thus $v_{k+1} = \sum_{i=2}^{k} \beta_i v_i$ with unique β_i. Hence $\alpha_1 = 0$ and, similarly, $\alpha_j = 0$ for all j such that $v_j \notin U$. Thus v_{k+1} is either null or linearly dependent on the remaining $v_i \in U$. Q. E. D.

Let $\mu_1, \ldots, \mu_n$ be any non-zero numbers related to a given $n \times n$ matrix Y be the ordering condition that $\delta_\nu(Y) \neq 0$, $\nu = 1, \ldots, n$, but for every μ_k and σ satisfying $|\mu_k| > |\mu_j|$ and $\sigma_i = i$, $i \leq j-1$, $\sigma_j = k$ then $\det(\underline{Y}_j^{\sigma}) = 0$. For

$\rho \in Z_{n,j}$ let μ^{ρ} denote $\mu_{\rho_1} \cdots \mu_{\rho_j}$. We can now state

LEMMA 4. <u>Let Y be a $n \times n$ matrix related to non-zero numbers $\mu_1, \ldots, \mu_n$ by the ordering condition given above. For $j = 1, \ldots, n$ and $\sigma \in Z_{n,j}$ the following statement holds. If $\det(Y_{\underline{j}}^{\sigma}) \neq 0$, $\sigma \neq \underline{j}$ then $|\mu^{\sigma}| \leq |\mu^{\underline{j}}|$ with equality occurring only if for each $\sigma_m > j$ there exists $\ell \leq j$ such that $|\mu_{\sigma_m}| = |\mu_{\ell}|$.</u>

Proof. For $j = 1, \det(Y_{\underline{j}}^{\sigma}) = y_{\sigma_1}$ and, by the ordering condition, $y_{\sigma_1} \neq 0$ implies $|\mu_{\sigma}| \leq |\mu_1|$. Thus the lemma is true for $j = 1$; we now assume it to hold for $j = k < n$.

For $\sigma \in Z_{n,k+1}$ let $\sigma(i)$ denote σ without the element σ_i. Let r_{σ_ν} and $\tilde{r}_{\sigma_\nu}$ denote row σ_ν of the matrices $Y_{\underline{k}}^{\sigma}$ and $Y_{\underline{k+1}}^{\sigma}$. To prove that the lemma holds for $j = k+1$ we assume that $\det(Y_{\underline{k+1}}^{\sigma}) \neq 0$, $\sigma \neq \underline{k+1}$. Let $S = \left\{\sigma_\nu : \det(Y_{\underline{k}}^{\sigma(\nu)}) \neq 0\right\}$.

By Lemma 3 the set $\left\{r_{\sigma_i} : \sigma_i \in S\right\}$ is linearly dependent. Also, if $|\mu_{\sigma_i}| > |\mu_{k+1}|$ for each $\sigma_i \in S$ then, by the ordering condition, $\tilde{r}_{\sigma_i}$ is linearly dependent on the independent set $\left\{\tilde{r}_\nu : \nu = 1, \ldots, k\right\}$. Thus there are unique α_{ij} such that

(*) $$\tilde{r}_{\sigma_i} = \sum_{j=1} a_{ij}\tilde{r}_j \ , \quad \sigma_i \in S \ .$$

Since (*) holds, a fortiori, with r_ν in place of $\tilde{r}_\nu$ it follows that the linear dependence of $\left\{r_{\sigma_i} : \sigma_i \in S\right\}$ implies the linear dependence of $\left\{\tilde{r}_{\sigma_i} : \sigma_i \in S\right\}$. This contradicts the hypothesis $\det(Y^{\sigma}_{\underline{k+1}}) \neq 0$ and so we cannot have $|\mu_{\sigma_i}|>|\mu_{k+1}|$ for all $\sigma_i \in S$.

By hypotheses $|\mu^{\sigma(i)}|\leq|\mu^{\underline{k}}|\ \forall\ \sigma_i \in S$. If $|\mu^{\sigma}|>|\mu^{\underline{k+1}}|$ then $|\mu_{\sigma_i}|>|\mu_{k+1}|\ \forall \sigma_i \in S$. Hence $|\mu^{\sigma}|\leq|\mu^{\underline{k+1}}|$ as was to be proved. We now examine the case of equality.

If $|\mu^{\sigma}| = |\mu^{\underline{k+1}}|$ and $|\mu^{\sigma(i)}|<|\mu^{\underline{k}}|\ \forall \sigma_i \in S$ then again $|\mu_{\sigma_i}|>|\mu_{k+1}|\ \forall \sigma_i \in S$. Hence for at least one $\sigma_i \in S$ we must have $|\mu^{\sigma(i)}| = |\mu^{\underline{k}}|$ and so, by hypothesis, either (a) $\sigma(i) = \underline{k}$ or (b) for each $\sigma_m \in \sigma(i)$, $\sigma_m > k$ there exists $\ell \leq k$ such that $|\mu_{\sigma_m}| = |\mu_\ell|$.

In both cases $|\mu_{\sigma_i}| = |\mu_{k+1}|$.

If (a) holds then $\sigma_i > k+1$ since $\sigma \neq \underline{k+1}$ and $\sigma_p \leq k$, $p \neq i$. If (b) holds then, a fortiori, $|\mu_{\sigma_m}| = |\mu_\ell|$ for $\sigma_m \in \sigma(i)$, $\sigma_m > k+1$. If $\sigma_i > k+1$ then,

since $|\mu_{\sigma_i}| = |\mu_{k+1}|$, the lemma is proved for $j = k+1$ in both case (a) and case (b).

By the principle of finite induction the lemma holds for all j for which it is meaningful, i.e. $j = 1,\ldots,n$.

COROLLARY. <u>If</u> $|\mu_i| \neq |\mu_j|$, $i \neq j$ <u>then</u> $|\mu^\sigma| > |\mu^j|$ <u>implies</u> $\det(Y_j^\sigma) = 0$.

If the matrix **A** has eigenvalues of distinct modulus and we order them with respect to Y as described above then the proof of Theorem 3 remains valid if we substitute the phrase "by the corollary of Lemma 4" for the phrase "hence by (i)" in the two places in which it occurs. Moreover r_j must be interpreted not as $|\lambda_{j+1}/\lambda_j|$ but as $|\lambda_j'/\lambda_j|$ where λ_j' is the eigenvalue of maximal modulus less then $|\lambda_j|$.

Thus the conclusion of Theorem 3 is valid for non-singular matrices with eigenvalues of distinct modulus.

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